

Kohonen and counterpropagation artificial neural networks in analytical chemistry

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Abstract

The principles of the Kohonen and counterpropagation artificial neural network (K-ANN and CP-ANN) learning strategy is described. The use of both methods (with the emphasis on CP-ANNs) is explained on several examples from analytical chemistry. The problems discussed in this presentation are: selection of a set of representative objects from a large number of multi-variate measurements, clustering of multi-variate experiments (multi-component analyses), generation of logical 'if-then' rules for an automatic decision making process, automatic evaluation of the quality of spectra based on their shape, spectra recording, quantitative decisions using weight maps, multi-variate modelling of a property, generation of multi-variate response surfaces from a generated CP-ANN model, and estimation of missing variable-values.

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